

Comment on "Analytic model of the energy spectrum of a graphene quantum dot in a perpendicular magnetic field"

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In recent work by Schnez et al. [PRB 78, 195427 (2008)], they studied the analytical model of the energy spectrum of a graphene quantum dot in a perpendicular magnetic field. In this comment we first point out that the results Eqs.(5), (6) and (11) presented by them in [1] are not reliable and then give our results.

The energy spectrum of graphene is linear at two inequivalent points in the Brillouin zone. The Hamiltonian reads

$$H = v_F(\vec{p} + e\vec{A}) \cdot \vec{\sigma} + \tau V(x, y)\sigma_z, \quad (1)$$

where v_F is Fermi velocity and $\tau = \pm 1$ distinguishes the two valleys K' and K and $\vec{\sigma} = (\sigma_x, \sigma_y)$ are Pauli's spin matrices.

Using the infinite-mass boundary, i.e., one has $V(r) = 0$ for $r \leq R$ and $V(r) = \infty$ for $r > R$. Thus for $V(r) = 0$, we can find the eigenvalue of the problem via $H\Psi = E\Psi$, where $\Psi = [\Psi_1(r, \varphi), \Psi_2(r, \varphi)]^T$ is the two-component spinor with $\Psi_1(r, \varphi) = e^{im\varphi}\chi_A$ and $\Psi_2(r, \varphi) = ie^{i(m+1)\varphi}\chi_B$, where $m = 0, \pm 1, \dots$. This boundary condition requires that $\Psi_2/\Psi_1 = i\tau e^{i\varphi}$ for circular confinement. The two components of the wave function χ_A and χ_B correspond to sublattice \mathcal{A} and \mathcal{B} . Substituting Ψ into the Dirac equation, we find the following coupled differential equations:

$$v_F \frac{d\chi_B(r)}{dr} + v_F \left(\frac{m+1}{r} + \frac{eBr}{2} \right) \chi_B(r) = E\chi_A, \quad -v_F \frac{d\chi_A(r)}{dr} + v_F \left(\frac{m}{r} + \frac{eBr}{2} \right) \chi_A(r) = E\chi_B, \quad (2)$$

where we have used the Pauli matrices in cylindrical coordinates

$$\sigma^r = \begin{pmatrix} 0 & e^{-i\varphi} \\ e^{i\varphi} & 0 \end{pmatrix}, \quad \sigma^\varphi = i \begin{pmatrix} 0 & -e^{-i\varphi} \\ e^{i\varphi} & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (3)$$

From (2) we obtain the following differential equations

$$\begin{aligned} \frac{d^2\chi_A(r)}{dr^2} + \frac{1}{r} \frac{d\chi_A(r)}{dr} - \left(\frac{m^2}{r^2} + \frac{m+1}{l_B^2} - k^2 + \frac{r^2}{4l_B^4} \right) \chi_A(r) &= 0, \\ \frac{d^2\chi_B(r)}{dr^2} + \frac{1}{r} \frac{d\chi_B(r)}{dr} - \left(\frac{(m+1)^2}{r^2} + \frac{m}{l_B^2} - k^2 + \frac{r^2}{4l_B^4} \right) \chi_B(r) &= 0. \end{aligned} \quad (4)$$

where factor $1/k$ multiplied by equation $\chi_B(r)$ is removed and $l_B = (eB)^{-1/2}$ denotes the magnetic length and $k = E/v_F$. Equation (4) can be further modified as

$$\begin{aligned} \frac{d^2\chi_A(s)}{ds^2} + \frac{1}{s} \frac{d\chi_A(s)}{ds} - \left(\frac{m^2}{4s^2} + \frac{m+1}{4sl_B^2} - \frac{k^2}{4s} + \frac{1}{16l_B^4} \right) \chi_A(s) &= 0, \\ \frac{d^2\chi_B(s)}{ds^2} + \frac{1}{s} \frac{d\chi_B(s)}{ds} - \left(\frac{(m+1)^2}{4s^2} + \frac{m}{4sl_B^2} - \frac{k^2}{4s} + \frac{1}{16l_B^4} \right) \chi_B(s) &= 0, \end{aligned} \quad (5)$$

where $s = r^2$.

The authors in [1] found out the solutions with slightly different expressions

$$\begin{aligned} \chi_A(s) &= C_m s^{\frac{m}{2}} \exp\left(-\frac{s}{4l_B^2}\right) L\left(\frac{k^2 l_B^2}{2} - (m+1), m, \frac{s}{2l_B^2}\right), \\ \chi_B(s) &= \frac{1}{kl_B^2} C_m s^{\frac{m+1}{2}} \exp\left(-\frac{s}{4l_B^2}\right) \left[L\left(\frac{k^2 l_B^2}{2} - (m+1), m, \frac{s}{2l_B^2}\right) + L\left(\frac{k^2 l_B^2}{2} - (m+2), m+1, \frac{s}{2l_B^2}\right) \right], \end{aligned} \quad (6)$$

where $s = r^2$.

Using the boundary condition $\Psi_2(r, \varphi)/\Psi_1(r, \varphi) = i\tau e^{i\varphi}$, they got the energy expression

$$\left(1 - \tau \frac{kl_B}{R/l_B}\right) L\left(\frac{k^2 l_B^2}{2} - (m+1), m, \frac{R^2}{2l_B^2}\right) + L\left(\frac{k^2 l_B^2}{2} - (m+2), m+1, \frac{R^2}{2l_B^2}\right) = 0 \quad (7)$$

We have to point out that the solutions (6) are incorrect and consequently the energy level equation (7) is flawed. Let us list these crucial mistakes below.

1) Considering the positive and negative quantum number m which determines the behaviors of the wave function near the origin, the *correct* solutions should be written as

$$\chi_A(s) = C_m s^{\frac{|m|}{2}} \exp\left(-\frac{s}{4l_B^2}\right) {}_1F_1\left(a, |m|+1, \frac{s}{2l_B^2}\right), \quad \chi_B(s) = \frac{1}{k l_B^2} C_m s^{\frac{|m+1|}{2}} \exp\left(-\frac{s}{4l_B^2}\right) {}_1F_1\left(\alpha, 1+|m+1|, \frac{s}{2l_B^2}\right), \quad (8)$$

where $a = 1 + (m + |m|)/2 - k^2 l_B^2/2$ and $\alpha = (1 + m + |m+1|)/2 - k^2 l_B^2/2$. For $m \geq 0$, we have $a = \alpha = 1 + m - k^2 l_B^2/2$, but for $m < 0$, we have $a = \alpha = 1 - k^2 l_B^2/2$. This means that a or α is independent of the m for negative m .

2) For the *unconfined* system, i.e. in the limits $B \rightarrow 0$ and $R/l_B \rightarrow \infty$, the normalizability requires a or α to be a non-positive integer, $a = -n = 0, -1, -2, \dots$, which gives the Landau energy levels

$$E = \begin{cases} \pm v_F \sqrt{[2(n+1) + 2m]eB}, & m \geq 0, \\ \pm v_F \sqrt{2(n+1)eB}, & m < 0, \end{cases} \quad (9)$$

which can be unified as

$$E = \pm v_F \sqrt{[2(n+1) + m + |m|]eB}, \quad \hbar = 1. \quad (10)$$

This implies that the Landau levels are independent of the number m for the case $m < 0$. Therefore, the Landau levels given by Eq.(11) of [1] are incorrect.

3) We note that for $a = -n$, the confluent hypergeometric function ${}_1F_1(-n, b+1, x)$ reduces to a generalized Laguerre polynomial $L(n, b, x)$. The authors of Ref. [1] made use of this relation to get Eqs. (5) and (6) of Ref. [1]. In fact, once considering an important identity $L(n, m, x) + L(n-1, m+1, x) = L(n, m+1, x)$ we will find that $\psi_2(r, \phi) \propto L(k^2 l_B^2/2 - (m+1), m+1, r^2/2l_B^2)$. Thus the implicit energy equation should have been given by

$$\tau \frac{kl_B}{R/l_B} L\left(n, m, \frac{R^2}{2l_B^2}\right) = L\left(n, m+1, \frac{R^2}{2l_B^2}\right). \quad (11)$$

Obviously, it is incorrect for the authors of Ref. [1] to obtain the energy spectrum by using Eq.(6) of Ref.[1]. This is because $n-1$ appeared in $L(n-1, m+1, k^2 l_B^2/2)$ if $n = k^2 l_B^2/2 - (m+1)$ ($m \geq 0$) was taken. This had to make them calculate the energy levels from quantum number $n = 1, \dots, 6$ but not from $n = 0, \dots, 5$ (see subsection C of Sec.II in page 195427-2 of Ref.[1]). Moreover, only for unconfined systems, it is possible to substitute ${}_1F_1(a, b+1, x)$ by $L(n, b, x)$ through taking $a = -n$. However, for confined system, i.e. for present graphene quantum dot, such a substitution is not allowed at all.

4) As a result, the correct energy level equations are given by

$$\begin{aligned} \tau \frac{kl_B}{R/l_B} {}_1F_1[a, m+1, R^2/2l_B^2] &= {}_1F_1[a, m+2, R^2/2l_B^2], & m \geq 0. \\ \tau \frac{kl_B}{R/l_B} {}_1F_1[\alpha, |m|+1, R^2/2l_B^2] &= {}_1F_1[\alpha, 1+|m+1|, R^2/2l_B^2], & m < 0. \end{aligned} \quad (12)$$

We plot curves of reduced energy spectrum correspond to magnetic field parameter $\beta = \frac{R^2}{2l_B^2}$ with reduced size $R = 1$ for $\tau = \pm 1$ and $m = 0, \pm 1, \pm 2, \pm 3, \pm 4$, respectively, in Fig. 1.

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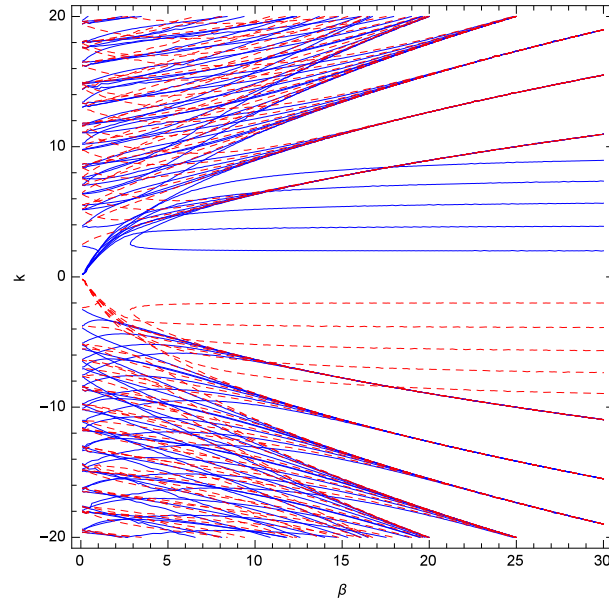


FIG. 1: (Color online) Reduced energy spectrum of a graphene quantum dot with reduced size $R = 1$ in a magnetic field. The energy levels corresponding to the $\tau = 1$ and $\tau = -1$ are shown, respectively, by the blue solid curves and the red dashed curves.

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